Random sampling locations for comparing a mean with a fixed threshold (parametric)

Summary
This report summarizes the sampling design used, associated statistical assumptions, as well as general guidelines for conducting post-sampling data analysis. Sampling plan components presented here include how many sampling locations to choose and where within the sampling area to collect those samples. The type of medium to sample (i.e., soil, groundwater, etc.) and how to analyze the samples (in-situ, fixed laboratory, etc.) are addressed in other sections of the sampling plan.

The following table summarizes the sampling design developed. A figure that shows sampling locations in the field and a table that lists sampling location coordinates are also provided below.

SUMMARY OF SAMPLING DESIGN	
Primary Objective of Design	Compare a site mean to a fixed threshold
Type of Sampling Design	Parametric
Sample Placement (Location) in the Field	Simple random sampling
Working (Null) Hypothesis	The mean value at the site exceeds the threshold
Formula for calculating number of sampling locations	Student's t-test
Calculated total number of samples	21
Number of samples on map [a]	23
Number of selected sample areas [b]	2
Specified sampling area [c]	188054.34 m^2
Total cost of sampling [d]	$11,500.00

[a] This number may differ from the calculated number because of 1) grid edge effects, 2) adding judgment samples, or 3) selecting or unselecting sample areas.
[b] The number of selected sample areas is the number of colored areas on the map of the site. These sample areas contain the locations where samples are collected.
[c] The sampling area is the total surface area of the selected colored sample areas on the map of the site.
[d] Including measurement analyses and fixed overhead costs. See the Cost of Sampling section for an explanation of the costs presented here.
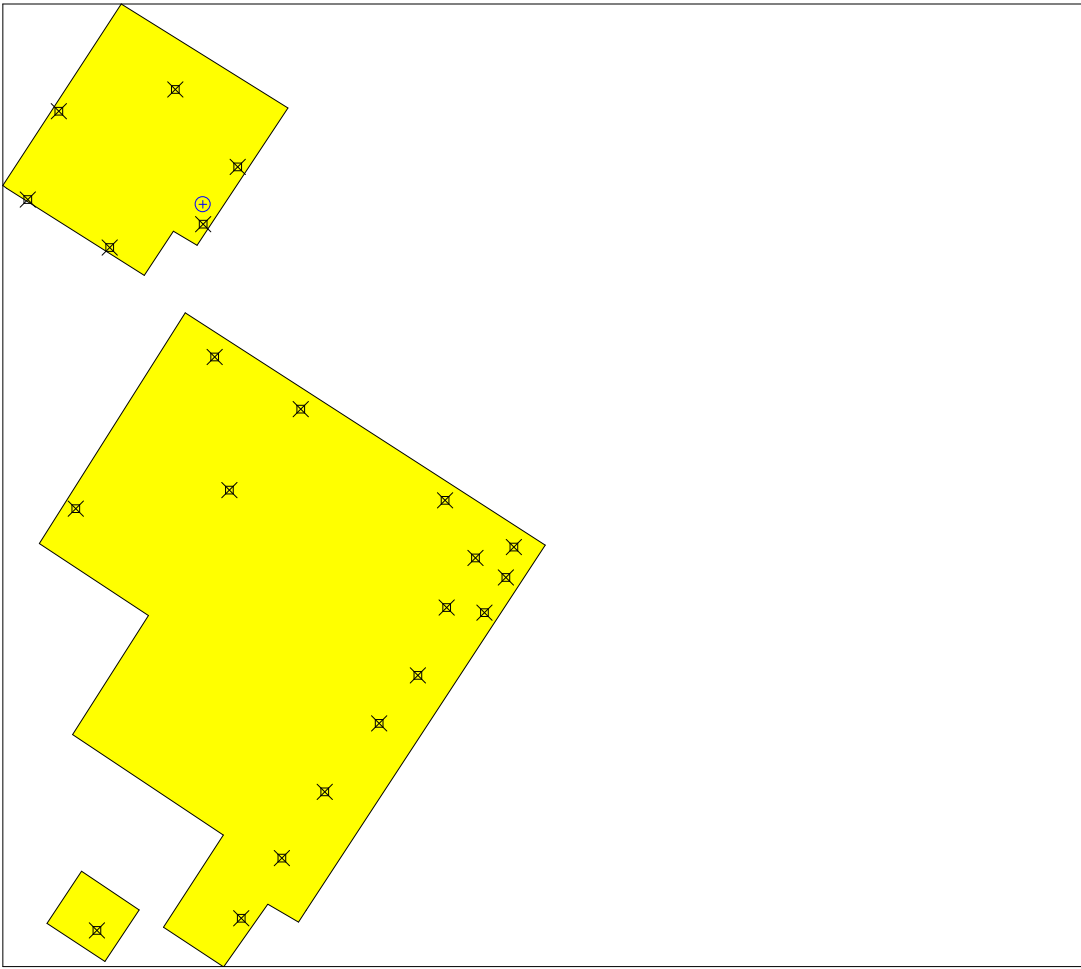
Area: Area 1					
X Coord	**Y Coord**	**Label**	**Value**	**Type**	**Historical**
679133.4290	3083306.3130	TW01-01	4.8	Manual	T
679104.2450	3083223.2620	TW01-02	5.1	Manual	T
679242.7260	3083326.5280	TW01-07	5.1	Manual	T
679181.2750	3083178.2880	TW01-08	6.2	Manual	T
679268.7700	3083200.3260	TW01-11	6.7	Manual	T
679301.1600	3083254.0340	TW01-12	4.8	Manual	T
679268.6582	3083218.6677	J-42SD	2.9	Random	

Area: Area 3					
X Coord	**Y Coord**	**Label**	**Value**	**Type**	**Historical**
679532.9930	3082835.5820	J-42SD	2.9	Manual	T
679552.9590	3082868.6600	J-43SD	2.7	Manual	T
679149.4920	3082933.0980	TW01-13	3.5	Manual	T
679279.7760	3083075.6320	TW01-14	2.7	Manual	T
679293.5600	3082950.4980	TW01-17	2.9	Manual	T
679360.5700	3083026.4980	TW01-18	2.7	Manual	T

679169.0760	3082537.3510	TW01-27	3.5	Manual	T
679495.8840	3082940.9730	TW01-33	3.7	Manual	T
679304.6530	3082548.6880	TW01-34	4.2	Manual	T
679342.7410	3082605.3190	TW01-35	4.8	Manual	T
679382.8900	3082667.5270	TW01-36	2.7	Manual	T
679433.9450	3082731.6820	TW01-37	2.7	Manual	T
679470.3570	3082776.7350	TW01-38	2.7	Manual	T
679497.3310	3082840.3960	TW01-39	2.7	Manual	T
679524.3310	3082886.8990	TW01-40	2.7	Manual	T
679560.6110	3082897.2580	TW01-41	4.1	Manual	T

Primary Sampling Objective
The primary purpose of sampling at this site is to compare a mean value with a fixed threshold. The working hypothesis (or 'null' hypothesis) is that the mean value at the site is equal to or exceeds the threshold. The alternative hypothesis is that the mean value is less than the threshold. VSP calculates the number of samples required to reject the null hypothesis in favor of the alternative hypothesis, given a selected sampling approach and inputs to the associated equation.

Selected Sampling Approach
A parametric random sampling approach was used to determine the number of samples and to specify sampling locations. A parametric formula was chosen because the conceptual model and historical information (e.g., historical data from this site or a very similar site) indicate that parametric assumptions are reasonable. These assumptions will be examined in post-sampling data analysis.

Both parametric and non-parametric approaches rely on assumptions about the population. However, non-parametric approaches typically require fewer assumptions and allow for more uncertainty about the statistical distribution of values at the site. The trade-off is that if the parametric assumptions are valid, the required number of samples is usually less than the number of samples required by non-parametric approaches.

Locating the sample points randomly provides data that are separated by many distances, whereas systematic samples are all equidistant apart. Therefore, random sampling provides more information about the spatial structure of the potential contamination than systematic sampling does. As with systematic sampling, random sampling also provides information regarding the mean value, but there is the possibility that areas of the site will not be represented with the same frequency as if uniform grid sampling were performed.

Number of Total Samples: Calculation Equation and Inputs
The equation used to calculate the number of samples is based on a Student's t-test. For this site, the null hypothesis is rejected in favor of the alternative hypothesis if the sample mean is sufficiently smaller than the threshold. The number of samples to collect is calculated so that 1) there will be a high probability $(1-\beta)$ of rejecting the null hypothesis if the alternative hypothesis is true and 2) a low probability (α) of rejecting the null hypothesis if the null hypothesis is true.

The formula used to calculate the number of samples is:

$$n = \frac{S^2}{\Delta^2}\left(Z_{1-\alpha} + Z_{1-\beta}\right)^2 + 0.5 Z_{1-\alpha}^2$$

where
n is the number of samples,
S is the estimated standard deviation of the measured values including analytical error,
Δ is the width of the gray region,
α is the acceptable probability of incorrectly concluding the site mean is less than the threshold,
β is the acceptable probability of incorrectly concluding the site mean exceeds the threshold,
$Z_{1-\alpha}$ is the value of the standard normal distribution such that the proportion of the distribution less than $Z_{1-\alpha}$ is $1-\alpha$,
$Z_{1-\beta}$ is the value of the standard normal distribution such that the proportion of the distribution less than $Z_{1-\beta}$ is $1-\beta$.

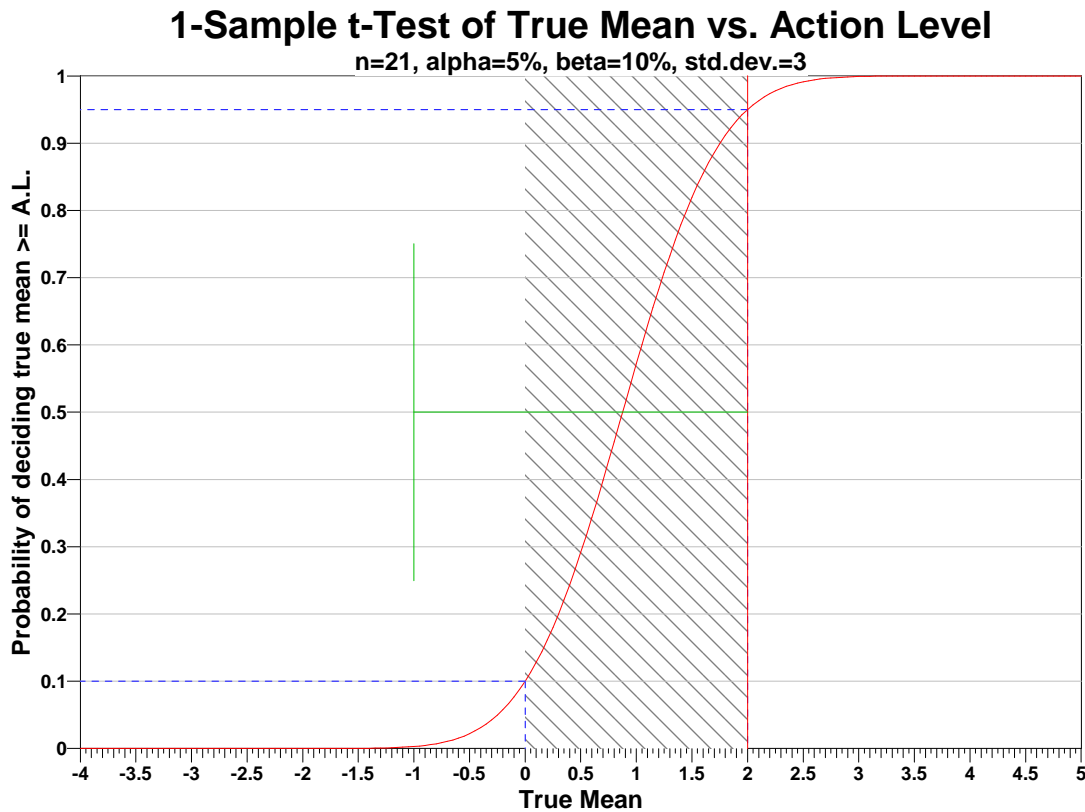The values of these inputs that result in the calculated number of sampling locations are:

Analyte	n	Parameter					
		S	Δ	α	β	$Z_{1-\alpha}$ [a]	$Z_{1-\beta}$ [b]
	21	3	2	0.05	0.1	1.64485	1.28155

[a] This value is automatically calculated by VSP based upon the user defined value of α.
[b] This value is automatically calculated by VSP based upon the user defined value of β.

The following figure is a performance goal diagram, described in EPA's QA/G-4 guidance (EPA, 2000). It shows the probability of concluding the sample area is dirty on the vertical axis versus a range of possible true mean values for the site on the horizontal axis. This graph contains all of the inputs to the number of samples equation and pictorially represents the calculation.

The red vertical line is shown at the threshold (action limit) on the horizontal axis. The width of the gray shaded area is equal to Δ; the upper horizontal dashed blue line is positioned at 1-α on the vertical axis; the lower horizontal dashed blue line is positioned at β on the vertical axis. The vertical green line is positioned at one standard deviation below the threshold. The shape of the red curve corresponds to the estimates of variability. The calculated number of samples results in the curve that passes through the lower bound of Δ at β and the upper bound of Δ at 1-α. If any of the inputs change, the number of samples that result in the correct curve changes.

1-Sample t-Test of True Mean vs. Action Level
n=21, alpha=5%, beta=10%, std.dev.=3

Probability of deciding true mean >= A.L. (vertical axis)
True Mean (horizontal axis)

Statistical Assumptions
The assumptions associated with the formulas for computing the number of samples are:
1.   the sample mean is normally distributed (this happens if the data are roughly symmetric and the sample size is 30 or more; for skewed data sets, additional samples are required for the sample mean to be normally distributed),
2.   the variance estimate, S^2, is reasonable and representative of the population being sampled,
3.   the population values are not spatially or temporally correlated, and
4.   the sampling locations will be selected randomly.
The first three assumptions will be assessed in a post data collection analysis. The last assumption is valid because the sample locations were selected using a random process.

Sensitivity Analysis
The sensitivity of the calculation of number of samples was explored by varying the standard deviation, lower bound of gray region (% of action level), beta (%), probability of mistakenly concluding that μ > action level and alpha (%), probability of mistakenly concluding that μ < action level and examining the resulting changes in the number of samples. The following table shows the results of this analysis.

AL=2		Number of Samples					
		α=5		α=10		α=15	
		s=6	s=3	s=6	s=3	s=6	s=3
LBGR=90	β=5	9742	2437	7709	1928	6471	1619
	β=10	7709	1929	5914	1479	4837	1210
	β=15	6472	1619	4837	1210	3868	968
LBGR=80	β=5	2437	611	1928	483	1619	405
	β=10	1929	484	1479	371	1210	303
	β=15	1619	406	1210	304	968	243
LBGR=70	β=5	1084	272	858	215	720	181
	β=10	858	216	658	166	538	135
	β=15	721	182	539	136	431	108

s = Standard Deviation
LBGR = Lower Bound of Gray Region (% of Action Level)
β = Beta (%), Probability of mistakenly concluding that μ > action level
α = Alpha (%), Probability of mistakenly concluding that μ < action level
AL = Action Level (Threshold)

Cost of Sampling
The total cost of the completed sampling program depends on several cost inputs, some of which are fixed, and others that are based on the number of samples collected and measured. Based on the numbers of samples determined above, the estimated total cost of sampling and analysis at this site is $11,500.00, which averages out to a per sample cost of $547.62. The following table summarizes the inputs and resulting cost estimates.

COST INFORMATION			
Cost Details	Per Analysis	Per Sample	21 Samples
Field collection costs		$100.00	$2,100.00
Analytical costs	$400.00	$400.00	$8,400.00
Sum of Field & Analytical costs		**$500.00**	**$10,500.00**
Fixed planning and validation costs			$1,000.00
Total cost			**$11,500.00**

Data Analysis
The following data points were entered by the user for analysis.

Rank	1	2	3	4	5	6	7	8	9	10
0	2.7	2.7	2.7	2.7	2.7	2.7	2.7	2.7	2.9	2.9
10	2.9	3.5	3.5	3.7	4.1	4.2	4.8	4.8	4.8	5.1
20	5.1	6.2	6.7							

SUMMARY STATISTICS

n	23
Min	2.7
Max	6.7
Range	4
Mean	3.7739
Median	3.5
Variance	1.5038
StdDev	1.2263
Std Error	0.2557
Skewness	0.95556
Interquartile Range	2.1

Percentiles								
1%	5%	10%	25%	50%	75%	90%	95%	99%
2.7	2.7	2.7	2.7	3.5	4.8	5.76	6.6	6.7

Outlier Test
Dixon's extreme value test was performed to test whether the lowest value is a statistical outlier. The test was conducted at the 5% significance level.

Data should not be excluded from analysis solely on the basis of the results of this or any other statistical test. If any values are flagged as possible outliers, further investigation is recommended to determine whether there is a plausible explanation that justifies removing or replacing them.

DIXON'S OUTLIER TEST	
Dixon Test Statistic	0
Dixon 5% Critical Value	0.421

The calculated test statistic does not exceed the critical value, so the test cannot reject the null hypothesis that there are no outliers in the data, and concludes that the minimum value 2.7 is not an outlier at the 5% significance level.

A normal distribution test indicated that the data do not appear to be normally distributed, so further investigation is recommended before using the results of this test. Because Dixon's test can be used only when the data without the suspected outlier are approximately normally distributed, a Shapiro-Wilk test for normality was performed at a 5% significance level.

NORMAL DISTRIBUTION TEST (excluding outliers)	
Shapiro-Wilk Test Statistic	0.8488
Shapiro-Wilk 5% Critical Value	0.911

The calculated Shapiro-Wilk test statistic is less than the 5% Shapiro-Wilk critical value, so the test rejects the hypothesis that the data are normal and concludes that the data, excluding the minimum value 2.7, do not appear to follow a normal distribution at the 5% level of significance. Dixon's test may not be appropriate if the assumption of normally distributed data is not justified for this data set. Examine the Q-Q plot displayed below to further assess the normality of the data.

Data Plots
Graphical displays of the data are shown below.

The Histogram is a plot of the fraction of the n observed data that fall within specified data "bins." A histogram is generated by dividing the x axis (range of the observed data values) into "bins" and displaying the number of data in each bin as the height of a bar for the bin. The area of the bar is the fraction of the n data values that lie within the bin. The

sum of the fractions for all bins equals one. A histogram is used to assess how the n data are distributed (spread) over their range of values. If the histogram is more or less symmetric and bell shaped, then the data may be normally distributed.

The Box and Whiskers plot is composed of a central box divided by a line, and with two lines extending out from the box, called the "whiskers". The line through the box is drawn at the median of the n data observed. The two ends of the box represent the 25th and 75th percentiles of the n data values, which are also called the lower and upper quartiles, respectively, of the data set. The sample mean (mean of the n data) is shown as a "+" sign. The upper whisker extends to the largest data value that is less than the upper quartile plus 1.5 times the interquartile range (upper quartile minus the lower quartile). The lower whisker extends to the smallest data value that is greater than the lower quartile minus 1.5 times the interquartile range. Extreme data values (greater or smaller than the ends of the whiskers) are plotted individually as blue Xs. A Box and Whiskers plot is used to assess the symmetry of the distribution of the data set. If the distribution is symmetrical, the box is divided into two equal halves by the median, the whiskers will be the same length, and the number of extreme data points will be distributed equally on either end of the plot.

The Q-Q plot graphs the quantiles of a set of n data against the quantiles of a specific distribution. We show here only the Q-Q plot for an assumed normal distribution. The pth quantile of a distribution of data is the data value, x_n, for which a fraction p of the distribution is less than x_n. If the data plotted on the normal distribution Q-Q plot closely follow a straight line, even at the ends of the line, then the data may be assumed to be normally distributed. If the data points deviate substantially from a linear line, then the data are not normally distributed.
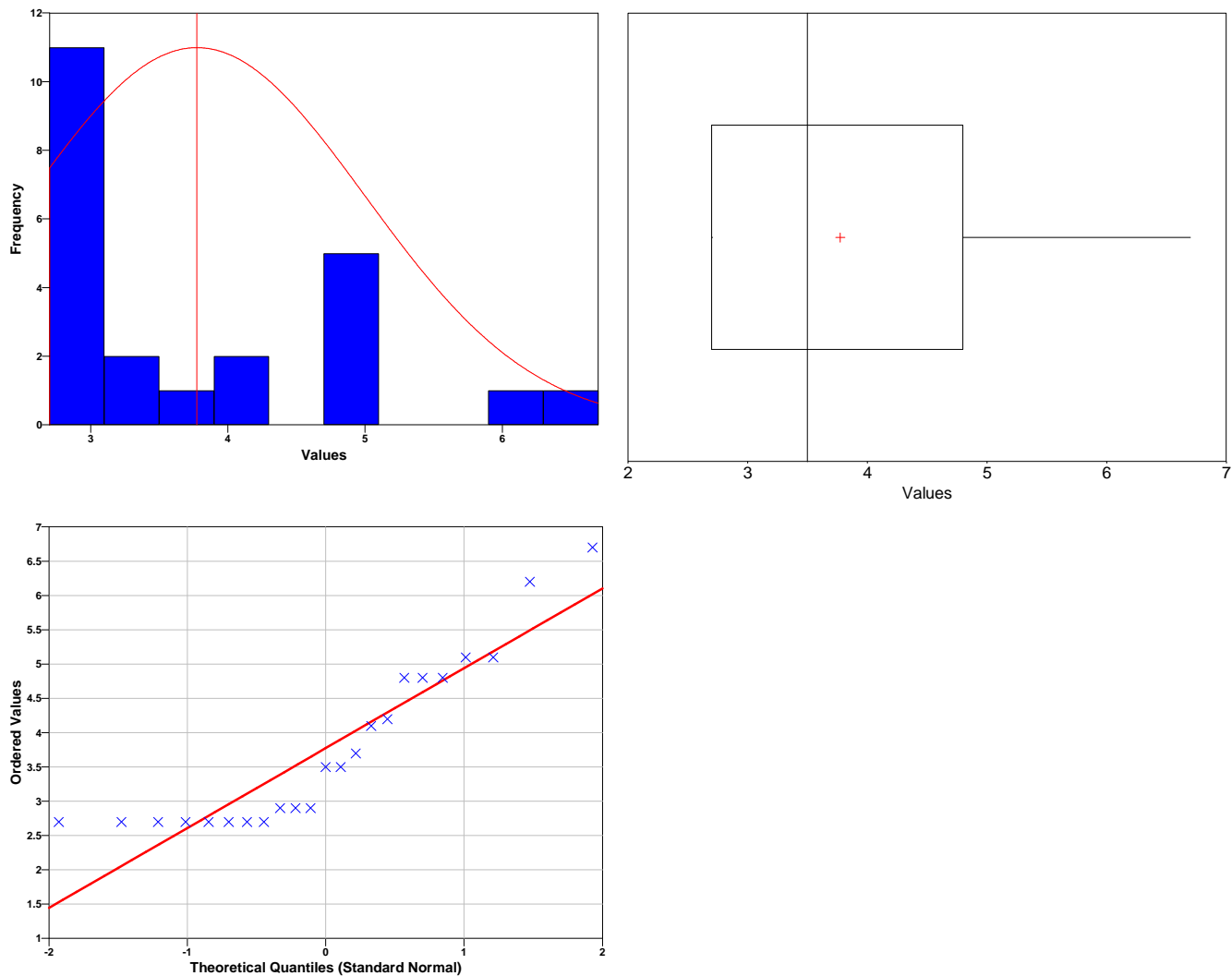
For more information on these plots consult Guidance for Data Quality Assessment, EPA QA/G-9, pgs 2.3-1 through 2.3-12. (http://www.epa.gov/quality/qa-docs.html).

Tests
A goodness-of-fit test was performed to test whether the data set had been drawn from an underlying normal distribution.

The Shapiro-Wilk (SW) test was used to test the null hypothesis that the data are normally distributed. The test was conducted at the 5% significance level, i.e., the probability the test incorrectly rejects the null hypothesis was set at 0.05.

NORMAL DISTRIBUTION TEST	
Shapiro-Wilk Test Statistic	0.834
Shapiro-Wilk 5% Critical Value	0.914

The calculated SW test statistic is less than the 5% Shapiro-Wilk critical value, so we can reject the hypothesis that the data are normal, or in other words the data do not appear to follow a normal distribution at the 5% level of significance. The Q-Q plot displayed above should be used to further assess the normality of the data.

Upper Confidence Limit on the True Mean
Two methods were used to compute the upper confidence limit (UCL) on the mean. The first is a parametric method that assumes a normal distribution. The second is the Chebyshev method, which requires no distributional assumption.

UCLs ON THE MEAN	
95% Parametric UCL	4.213
95% Non-Parametric (Chebyshev) UCL	4.888

Because the data do not appear to be normally distributed according to the goodness-of-fit test performed above, the non-parametric UCL (4.888) may be a more accurate upper confidence limit on the true mean.

One-Sample t-Test
A one-sample t-test was performed to compare the sample mean to the action level. The null hypothesis used is that the true mean equals or exceeds the action level (AL). The t-test was conducted at the 5% significance level. The sample value t was computed using the following equation:

$$t = \frac{\bar{x} - AL}{SE}$$

where
x is the sample mean of the n=23 data,
AL is the action level or threshold (2),
SE is the standard error = (standard deviation) / (square root of n).

This t was then compared with the critical value $t_{0.95}$, where $t_{0.95}$ is the value of the t distribution with n-1=22 degrees of freedom for which the proportion of the distribution to the left of $t_{0.95}$ is 0.95. The null hypothesis will be rejected if $t < -t_{0.95}$.

ONE-SAMPLE t-TEST		
t-statistic	Critical Value $t_{0.95}$	Null Hypothesis
6.9374	1.7171	Reject

The test rejected the null hypothesis that the mean value at the site exceeds the threshold, therefore conclude the true mean is less than the threshold.

Because the data do not appear to be normally distributed, the MARSSIM Sign Test might be preferred over the One Sample t-Test. The following table represents the results of the MARSSIM Sign Test using the current data:

MARSSIM Sign Test		
Test Statistic (S+)	95% Critical Value	Null Hypothesis
0	15	Cannot Reject
Note: There may not be enough data to reject the null hypothesis (and conclude site is clean) with 95% confidence using the MARSSIM sign test.		